Automated Implementation

The various techniques, methods, and aspects of the instant invention can be implemented in part or in whole using computer-based systems and methods. Additionally, computer-based systems and methods can be used to augment or enhance the functionality described above, increase the speed at which the functions can be performed, and provide additional features and aspects as a part of or in addition to those of the present invention as described herein.

The various embodiments, aspects, and features of the invention described above can be implemented using hardware, software, or a combination thereof, and can be implemented using a computing system having one or more processors. In alternative embodiments, these elements are implemented using a processor-based system capable of carrying out the functionality described with respect thereto. Typically, a computer includes one or more processors. The processor(s) is(are) connected to a communication bus. Various software embodiments are described in terms of this example computer system. The embodiments, features, and functionality of the invention are not dependent on a particular computer system or processor architecture or on a particular operating system, algorithm, or software. In fact, given the instant description, it will be apparent to a person of ordinary skill in the relevant art how to implement the invention using other computer or processor systems and/or architectures.

In some embodiments, a processor-based system can include a main memory, such as a random access memory (RAM), and can also include one or more secondary memories. The secondary memory can include, for example, a hard disk drive and/or a removable storage drive, *e.g.*, a floppy disk drive, a magnetic tape drive, an optical disk drive, *etc*. The removable storage drive reads from and/or writes to a removable storage medium, such as a floppy disk, magnetic tape, optical disk, *etc.* that can be read by and/or written to by a removable storage drive. The removable storage media includes a computer usable storage medium having stored

therein computer software and/or data. Other alternative embodiments and configurations can also be employed.

A computer system according to the invention can also include a communications interface to allow software and data to be transferred between computer system and external devices. Examples of communications interfaces include modems, network interfaces (such as, for example, an Ethernet card), a communications port, a PCMCIA slot and card, *etc*. Software and data transferred via communications interface 524 are in the form of signals which can be electronic, electromagnetic, optical, or other signals capable of being received by the communications interface. These signals are provided to the communications interface via a channel that carries signals and can be implemented using a wireless medium, wire or cable, fiber optics, or other communications media.

In this document, the terms "computer program medium" and "computer usable medium" are used to generally refer to media such as a removable storage device, a disk capable of installation in a disk drive, and signals on channels. These computer program products provide software or program instructions to the computer system.

Computer programs (also called computer control logic) can be stored in a memory. Computer programs can also be received via a communications interface. Such computer programs, when executed, enable the computer system to perform the features of the present invention. In particular, the computer programs, when executed, enable the processor(s) to perform the features of the present invention. Accordingly, such computer programs represent controllers of the computer system.

EXAMPLES

The following examples are provided to illustrate the practice of preferred embodiments of the instant invention, and in no way limit the scope of the invention.

Example 1

SICHO-Mediated Folding of 8 Representative Proteins

The test set employed in this work is representative of single domain water-soluble proteins[40] and consists of the following proteins that were previously studied[6] in the CAPLUS model: the small structured protein fragment of 6pti, chosen for comparison with the work of Smith-Brown *et al.*, the all-α protein myoglobin (1mbs), the α/β motifs of protein G, thioredoxin, flavodoxin, and an all-β protein, 1 pcy. In addition, the folding of a 247-residue TIM barrel, Atim, and the β-protein 4fab was also examined. The set of constraints used in these studies have been reported previously,[6] but only in those cases where the studied protein is the same. When a smaller number of constraints are used, they were randomly chosen from the larger constraint set. For the two proteins not studied previously, the set of long-range constraints employed appears in Tables II and III, below. The short-range constraints, as before, come from the three-letter code of the DSSP assignment[37] of the native secondary structure, and are as described above.

TABLE II. Tertiary Constraint Lists for 4fab

27 constraints		16 constraints
1 PRO	ASN-100	xx
4 GLN	MET-95	
8 THR	PRO-107	xx
8 ILE	PRO-21	xx
11 ILE	LEU-21	
11 THR	LEU-107	
15 ILE	LEU-111	xx
19 LEU	ALA-109	xx
20 LYS	SER-79	xx
23 TRP	SER-40	
23 PHE	SER-76	
29 HIS	LEU-98	xx
34 LYS	GLY-55	
37 LYS	TYR-55	
39 TYR	ARG-54	xx
39 SER	ARG-94	xx
40 LEU	TRP-52	xx
44 GLY	LYS-89	xx